

Symmetric Perry conjugate gradient method

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Abstract A family of new conjugate gradient methods is proposed based on Perry's idea, which satisfies the descent property or the sufficient descent property for any line search. In addition, based on the scaling technology and the restarting strategy, a family of scaling symmetric Perry conjugate gradient methods with restarting procedures is presented. The memoryless BFGS method and the SCALCG method are the special forms of the two families of new methods, respectively. Moreover, several concrete new algorithms are suggested. Under Wolfe line searches, the global convergence of the two families of the new methods is proven by the spectral analysis for uniformly convex functions and nonconvex functions. The preliminary numerical comparisons with CG_DESCENT and SCALCG algorithms show that these new algorithms are very effective algorithms for the large-scale unconstrained optimization problems. Finally, a remark for further research is suggested.

Keywords Conjugate gradient method · Descent property · Spectral analysis · Global convergence

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1 Introduction

The classical conjugate gradient (CG) method with line search is as follows:

$$x_{k+1} = x_k + \alpha_k d_k, \quad (1)$$

where the directions d_k is given by

$$\begin{cases} d_1 = -g_1, \\ d_{k+1} = -g_{k+1} + \beta_k d_k, \quad \forall k \geq 1, \end{cases} \quad (2)$$

where $g_k = g(x_k) = \nabla f(x_k)$. The different choices for the parameter β_k correspond to different CG methods, such as HS method [15], FR method [7], PRP method [22, 23], LS method [16], PRP⁺ method [8], DY method [5] and so on. On the history of the conjugate gradient method, there are several survey articles, such as [11].

In [17], the Perry conjugate gradient algorithm [21] was generalized and the line search directions were formulated as follows:

$$\begin{cases} d_1 = -g_1, \\ d_{k+1} = -P_{k+1}g_{k+1} = -g_{k+1} + \frac{y_k^T g_{k+1}}{s_k^T y_k} s_k - \sigma \frac{s_k^T g_{k+1}}{y_k^T u_k} u_k, \quad \forall k > 1, \end{cases} \quad (3)$$

where $s_k = x_{k+1} - x_k = \alpha_k d_k$, $y_k = g_{k+1} - g_k$, α_k is the steplength of the line search and σ is a preset parameter,

$$P_{k+1} = \left(I - \frac{s_k y_k^T}{s_k^T y_k} + \sigma \frac{u_k s_k^T}{y_k^T u_k} \right), \quad (4)$$

which is called Perry iteration matrix, and the vector u_k is any vector in \mathbb{R}^n such that $y_k^T u_k \neq 0$. In the paper [17], the case $u_k = y_k$ was discussed. When $u_k = s_k$, the CG_DESCENT algorithm [10–12] can be deduced and the D-L method [4] can be derived from the restriction $\sigma > 0$. Recently, we also studied the case $u_k = s_k$ in [19] and presented a RSPDCGs algorithm.

In this paper, a family of symmetric Perry conjugate gradient methods is proposed, that is, the line search directions are formulated by

$$\begin{cases} d_1 = -g_1, \\ d_{k+1} = -Q_{k+1}g_{k+1} = -g_{k+1} + \beta_k d_k + \gamma_k y_k, \\ \quad = -g_{k+1} + \frac{s_k^T g_{k+1}}{s_k^T y_k} y_k + \left[\frac{y_k^T g_{k+1}}{s_k^T y_k} - \left(\sigma + \frac{y_k^T y_k}{s_k^T y_k} \right) \frac{s_k^T g_{k+1}}{s_k^T y_k} \right] s_k, \quad \forall k \geq 1 \end{cases} \quad (5)$$

where $\beta_k = \frac{y_k^T g_{k+1}}{d_k^T y_k} - (\alpha_k \sigma + \frac{y_k^T y_k}{d_k^T y_k}) \frac{d_k^T g_{k+1}}{d_k^T y_k}$, $\gamma_k = \frac{d_k^T g_{k+1}}{d_k^T y_k}$ and

$$Q_{k+1} = I - \frac{s_k y_k^T + y_k s_k^T}{s_k^T y_k} + \left(\sigma + \frac{y_k^T y_k}{s_k^T y_k} \right) \frac{s_k s_k^T}{s_k^T y_k}, \quad (6)$$

which is called the symmetric Perry iteration matrix. When $\sigma y_k^T s_k > 0$, for any line search, the directions defined by (5) satisfy the descent property [1]

$$d_{k+1}^T g_{k+1} < 0, \quad (7)$$

or the sufficient descent property [8]

$$d_{k+1}^T g_{k+1} \leq -c_0 \|g_{k+1}\|^2 \quad (c_0 > 0). \quad (8)$$

This paper is organized as follows. In Sect. 2, first, the family of the symmetric Perry conjugate gradient methods is deduced. Then the spectra of the iteration matrix are analyzed, so, its sufficient descent property is proved and several concrete algorithms are proposed. In Sect. 3, the scaling technology and the restarting strategy are applied to the symmetric Perry conjugate gradient methods, thus, a family of scaling Perry conjugate gradient methods with restarting procedures is developed. In Sect. 4, the global convergence of the two families of the new methods with the Wolfe line searches is proven by the spectral analysis of the conjugate gradient iteration matrix. In Sect. 5, the preliminary numerical results are reported. A remark for further research is given in Sect. 6.

2 The symmetric Perry conjugate gradient method

In [21], A. Perry changed the CG update parameter β_k of the HS conjugate gradient method [15] into $\beta_k^P = \frac{(y_k - s_k)^T g_{k+1}}{y_k^T d_k}$, and formulated the line search directions

$$d_{k+1} = -g_{k+1} + \beta_k^P d_k = -Q_{k+1} g_{k+1}, \quad k = 1, 2, \dots,$$

and

$$y_k^T d_{k+1} = -s_k^T g_{k+1}, \quad (9)$$

where

$$Q_{k+1} = D_{k+1} + \frac{s_k s_k^T}{y_k^T s_k} \quad \text{and} \quad D_{k+1} = \left(I - \frac{s_k y_k^T}{s_k^T y_k} \right). \quad (10)$$

In [17], (10) and (9) were substituted by

$$Q_{k+1} = D_{k+1} + uv^T \quad (11)$$

and

$$y_k^T d_{k+1} = -\sigma s_k^T g_{k+1}, \quad (12)$$

respectively, where $u, v \in \mathbb{R}^n$ and σ is a parameter. Thus, it follows from (11), (12) and $d_{k+1} = -Q_{k+1} g_{k+1}$ that $(\sigma s_k - v y_k^T u)^T g_{k+1} = 0$, which yields $v = \frac{\sigma s_k}{y_k^T u}$. So,

$$Q_{k+1} = \left(I - \frac{s_k y_k^T}{s_k^T y_k} + \sigma \frac{u s_k^T}{y_k^T u} \right), \quad (13)$$

from which the generalized Perry conjugate gradient method ((1) and (3)) can be obtained [17].

In this paper, we choose a suitable u such that Q_{k+1} is a symmetric matrix, thus the line search directions d_k may satisfy (7) or (8). Let $Q_{k+1} = Q_{k+1}^T$, then

$$\left(\frac{y_k}{s_k^T y_k} + \sigma \frac{u}{y_k^T u} \right) s_k^T = s_k^T \left(\frac{y_k}{s_k^T y_k} + \sigma \frac{u}{y_k^T u} \right)^T.$$

Therefore, the vector u can be taken as

$$u = a \left(\frac{\sigma s_k^T y_k + y_k^T y_k}{(s_k^T y_k)^2} s_k - \frac{1}{s_k^T y_k} y_k \right) \quad (a \neq 0), \quad (14)$$

and $u^T y_k = a\sigma$. We note that the matrix Q_{k+1} defined by (13) is independent of the nonzero constant a , so, we can choose $a = 1$. Thus, from (13) and (14) we can obtain the matrix Q_{k+1} defined by (6).

The method formulated by (1) and (5) is called the symmetric Perry conjugate gradient method, denoted by SPCG. And the directions generated by (5) are called the symmetric Perry conjugate gradient directions, which will be proven to be descent directions in Sect. 2.2.

From the above discussions, a family of new nonlinear conjugate gradient algorithms can be obtained as follows:

Algorithm 1 (SPCG)

- Step 1. Give an initial point x_1 and $\varepsilon \geq 0$. Set $k = 1$.
- Step 2. Calculate $g_1 = g(x_1)$. If $\|g_1\| \leq \varepsilon$ then stop, otherwise let $d_1 = -g_1$.
- Step 3. Calculate steplength α_k with line searches.
- Step 4. Set $x_{k+1} = x_k + \alpha_k d_k$.
- Step 5. Calculate $g_{k+1} = g(x_{k+1})$. If $\|g_{k+1}\| \leq \varepsilon$ then stop.
- Step 6. Calculate the directions d_{k+1} via (5) with different σ .
- Step 7. Set $k = k + 1$, then go to step 3.

Remark 1 In this paper, to ensure the convergence of the algorithm, we adopt the Wolfe line search strategies:

$$f(x_k + \alpha_k d_k) \leq f(x_k) + b_1 \alpha_k d_k^T g_k \quad (15)$$

and

$$d_k^T g(x_k + \alpha_k d_k) \geq b_2 d_k^T g_k, \quad (16)$$

where $0 < b_1 < b_2 < 1$. The stopping criterion, $\|g_k\| \leq \varepsilon$, can be changed into other forms. For the different choices of σ , several concrete forms of the algorithm will be discussed in the Sect. 2.2.

2.1 Spectral analysis

Here, we analyze the spectra of the Perry matrix and the symmetric Perry matrix.

Theorem 1 Let P_{k+1} be defined by (4). Then when $\sigma(y_k^T s_k) \neq 0$, P_{k+1} is a nonsingular matrix and the eigenvalues of P_{k+1} consist of 1 ($n - 2$ multiplicity), λ_1^{k+1} and λ_2^{k+1} , where

$$\lambda_1^{k+1} = \frac{1}{2} \left[\left(1 + \sigma \frac{s_k^T u_k}{y_k^T u_k} \right) - \sqrt{\left(1 + \sigma \frac{s_k^T u_k}{y_k^T u_k} \right)^2 - 4\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right] \quad (17)$$

and

$$\lambda_2^{k+1} = \frac{1}{2} \left[\left(1 + \sigma \frac{s_k^T u_k}{y_k^T u_k} \right) + \sqrt{\left(1 + \sigma \frac{s_k^T u_k}{y_k^T u_k} \right)^2 - 4\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right]. \quad (18)$$

Proof From the fundamental algebra formula

$$\det(I + xy^T + uv^T) = (1 + y^T x)(1 + v^T u) - (x^T v)(y^T u),$$

it follows that

$$\det(P_{k+1}) = \det\left(I - \frac{s_k y_k^T}{s_k^T y_k} + \frac{\sigma u_k s_k^T}{y_k^T u_k}\right) = \sigma \frac{s_k^T s_k}{y_k^T s_k}. \quad (19)$$

Therefore, the Perry matrix (4) is a nonsingular matrix when $\sigma y_k^T s_k \neq 0$.

Since $\forall \xi \in \text{span}\{s_k, y_k\}^\perp \subset \mathbb{R}^n$,

$$P_{k+1}\xi = \left(I - \frac{s_k y_k^T}{s_k^T y_k} + \sigma \frac{u_k s_k^T}{y_k^T u_k}\right)\xi = \xi - \frac{y_k^T \xi}{s_k^T y_k} s_k + \sigma \frac{s_k^T \xi}{y_k^T u_k} u_k = \xi,$$

the matrix P_{k+1} has the eigenvalue 1 ($n - 2$ multiplicity), corresponding to the eigenvectors $\xi \in \text{span}\{s_k, y_k\}^\perp$.

By the relationships between the trace and the eigenvalues of matrix and between the determinant and the eigenvalues of matrix, the other two eigenvalues are the roots of the following quadratic polynomial

$$\lambda^2 - \left(1 + \sigma \frac{s_k^T u_k}{y_k^T u_k}\right)\lambda + \sigma \frac{s_k^T s_k}{y_k^T s_k} = 0. \quad (20)$$

Thus, the other two eigenvalues are determined by (17) and (18), respectively. \square

According to Theorem 1, the following theorem for the symmetric Perry matrix Q_{k+1} defined by (6) can be deduced.

Theorem 2 Let $\lambda_{\min}^{(k+1)}$ and $\lambda_{\max}^{(k+1)}$ be the minimum and maximum eigenvalues of Q_{k+1} , respectively, where Q_{k+1} is defined by (6). If $\sigma(y_k^T s_k) > 0$, then

$$\lambda_{\min}^{(k+1)} = \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - \sqrt{\left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right)^2 - 4\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right], \quad (21)$$

$$\lambda_{\max}^{(k+1)} = \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} + \sqrt{\left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right)^2 - 4\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right], \quad (22)$$

$$\frac{\sigma y_k^T s_k}{y_k^T y_k + \sigma y_k^T s_k} \leq \lambda_{\min}^{(k+1)} \leq 1 \leq \omega_k \leq \lambda_{\max}^{(k+1)} \leq \omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \quad (23)$$

and

$$\lambda_{\min}^{(k+1)} \leq \sigma \frac{s_k^T s_k}{s_k^T y_k} \leq \max \left\{ \omega_k, \omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - 1 \right\} \leq \lambda_{\max}^{(k+1)}, \quad (24)$$

where $\omega_k = \frac{y_k^T y_k s_k^T s_k}{(s_k^T y_k)^2}$. Moreover, Q_{k+1} is a symmetric positive definite matrix when $\sigma(y_k^T s_k) > 0$.

Proof When $\sigma(y_k^T s_k) > 0$, from (14), (17), (18) and the following relations:

$$\left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right)^2 - 4\sigma \frac{s_k^T s_k}{y_k^T s_k} = \left(\omega_k - \sigma \frac{s_k^T s_k}{s_k^T y_k} \right)^2 + 4\sigma(\omega_k - 1) \frac{s_k^T s_k}{s_k^T y_k} \geq 0, \quad (25)$$

it can be proven that $\lambda_{\min}^{(k+1)}$ and $\lambda_{\max}^{(k+1)}$ are formulated by (21) and (22), respectively. Simple calculation claims that

$$\lambda_{\max}^{(k+1)} \leq \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} + \sqrt{\left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right)^2} \right] = \omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k}$$

and

$$\begin{aligned} \lambda_{\max}^{(k+1)} &= \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} + \sqrt{4(\omega_k - 1) + \left(\omega_k - 2 + \sigma \frac{s_k^T s_k}{y_k^T s_k} \right)^2} \right] \\ &\geq \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} + \left| \omega_k - 2 + \sigma \frac{s_k^T s_k}{y_k^T s_k} \right| \right]. \end{aligned} \quad (26)$$

So, the inequality (26) implies that

$$\lambda_{\max}^{(k+1)} \geq \omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - 1 \geq \sigma \frac{s_k^T s_k}{s_k^T y_k}.$$

In addition, it follows from (25) that

$$\lambda_{\max}^{(k+1)} \geq \frac{1}{2} \left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} + \left| \omega_k - \sigma \frac{s_k^T s_k}{s_k^T y_k} \right| \right) \geq \omega_k.$$

Therefore, $\lambda_{\max}^{(k+1)} \geq \max \{ \omega_k, \omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - 1 \} \geq \sigma \frac{s_k^T s_k}{s_k^T y_k}$.

Similarly,

$$\begin{aligned}\lambda_{\min}^{(k+1)} &= \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - \sqrt{\left(\omega_k - \sigma \frac{s_k^T s_k}{s_k^T y_k} \right)^2 + 4(\omega_k - 1) \sigma \frac{s_k^T s_k}{y_k^T s_k}} \right] \\ &\leq \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - \left| \omega_k - \sigma \frac{s_k^T s_k}{s_k^T y_k} \right| \right] \leq \sigma \frac{s_k^T s_k}{s_k^T y_k}\end{aligned}$$

and

$$\begin{aligned}\lambda_{\min}^{(k+1)} &= \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - \sqrt{4(\omega_k - 1) + \left(\omega_k - 2 + \sigma \frac{s_k^T s_k}{y_k^T s_k} \right)^2} \right] \\ &\leq \frac{1}{2} \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} - \left| \omega_k + \sigma \frac{s_k^T s_k}{y_k^T s_k} - 2 \right| \right] \leq 1.\end{aligned}$$

In the end, it follows from (20) that $\lambda_{\min}^{(k+1)} \lambda_{\max}^{(k+1)} = \sigma \frac{s_k^T s_k}{y_k^T s_k}$, which implies that

$$\lambda_{\min}^{(k+1)} = (\lambda_{\max}^{(k+1)})^{-1} \sigma \frac{s_k^T s_k}{y_k^T s_k} \geq \left(\omega_k + \sigma \frac{s_k^T s_k}{y_k^T s_k} \right)^{-1} \sigma \frac{s_k^T s_k}{y_k^T s_k} = \frac{\sigma y_k^T s_k}{y_k^T y_k + \sigma y_k^T s_k}.$$

Hence, (23) and (24) hold, which implies that Q_{k+1} is a symmetric positive definite matrix when $\sigma(y_k^T s_k) > 0$. \square

From the above theorem, we can easily obtain the following corollary.

Corollary 1 Let Q_{k+1} be defined by (6) and $\sigma(y_k^T s_k) > 0$. The spectral condition number of Q_{k+1} , $\kappa_2(Q_{k+1})$, is formulated by

$$\kappa_2(Q_{k+1}) = \left[\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} + \sqrt{\left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right)^2 - 4\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right]^2 / 4\sigma \frac{s_k^T s_k}{y_k^T s_k}. \quad (27)$$

Especially, $\kappa_2(Q_{k+1})$ arrives at the minimum, $(\sqrt{\omega_k} + \sqrt{\omega_k - 1})^2$, when $\sigma = \frac{y_k^T y_k}{s_k^T y_k}$.

Proof According to Theorem 2, (21) and (22) imply that (27) holds. Let

$$t = \left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right) / \left(2\sqrt{\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right), \quad (28)$$

then, according to (27), $\kappa_2(Q_{k+1})$ can be rewritten as follows:

$$\kappa_2(Q_{k+1}) = \psi(t) = (t + \sqrt{t^2 - 1})^2, \quad (29)$$

where $\psi(\cdot)$ is a strictly increasing function on $[1, +\infty)$. Note that

$$t \geq \left(2\sqrt{\omega_k} \sqrt{\sigma \frac{s_k^T s_k}{s_k^T y_k}} \right) / \left(2\sqrt{\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right) = \sqrt{\omega_k} \geq 1$$

and the above first inequality takes “=” if and only if $\omega_k = \sigma \frac{s_k^T s_k}{s_k^T y_k}$, namely, $\sigma = \frac{y_k^T y_k}{s_k^T y_k}$. Hence, the minimum of $\kappa_2(Q_{k+1})$ is $(\sqrt{\omega_k} + \sqrt{\omega_k - 1})^2$ when $\sigma = \frac{y_k^T y_k}{s_k^T y_k}$. \square

2.2 Descent property

For the SPCG method, Theorem 2 shows that the symmetric Perry conjugate gradient directions defined by (5) satisfy the descent property (7), when $\sigma y_k^T s_k > 0$. In fact,

$$d_{k+1}^T g_{k+1} = -g_{k+1}^T Q_{k+1} g_{k+1} \leq -\lambda_{\min}^{(k+1)} \|g_{k+1}\|^2 \leq -\frac{\sigma y_k^T s_k \|g_{k+1}\|^2}{y_k^T y_k + \sigma y_k^T s_k} < 0. \quad (30)$$

When $\sigma = 1$, Q_{k+1} , defined by (6), becomes

$$H_{k+1}^{\text{mBFGS}} = I - \frac{s_k y_k^T + y_k s_k^T}{s_k^T y_k} + \left(1 + \frac{y_k^T y_k}{s_k^T y_k}\right) \frac{s_k s_k^T}{s_k^T y_k}. \quad (31)$$

Thus, the method defined by (1) and (5) with $\sigma = 1$ is the famous memoryless BFGS quasi-Newton method [25], denoted by mBFGS.

According to (30), we let $\sigma = c \frac{y_k^T y_k}{s_k^T y_k}$, $c > 0$ and $s_k^T y_k \neq 0$, then it follows from (6) and (30) that

$$Q_{k+1}^{\text{SPD}} = \left(I - \frac{s_k y_k^T}{s_k^T y_k}\right) \left(I - \frac{y_k s_k^T}{s_k^T y_k}\right) + c \frac{y_k^T y_k}{s_k^T y_k} \frac{s_k s_k^T}{s_k^T y_k} \quad (32)$$

and

$$d_{k+1}^T g_{k+1} \leq -\frac{c}{1+c} \|g_{k+1}\|_2^2, \quad (33)$$

which shows that the directions defined by (5) with $\sigma = c \frac{y_k^T y_k}{s_k^T y_k}$ satisfy the sufficient descent property (8) for any functions and any line searches. Thus, the method defined by (1) and (5) with $\sigma = c \frac{y_k^T y_k}{s_k^T y_k}$ is called symmetric Perry descent conjugate gradient algorithm, denoted by SPDCG, or by SPDCG(c), to indicate the dependence on the positive constant c . Especially, due to Corollary 1, when $c = 1$, the method is called symmetric Perry descent conjugate gradient algorithm with optimal condition number, denoted by SPDOC. The corresponding iteration matrix is denoted by Q_{k+1}^{SPDOC} , i.e.

$$Q_{k+1}^{\text{SPDOC}} = \left(I - \frac{s_k y_k^T}{s_k^T y_k}\right) \left(I - \frac{y_k s_k^T}{s_k^T y_k}\right) + \frac{y_k^T y_k}{s_k^T y_k} \frac{s_k s_k^T}{s_k^T y_k}. \quad (34)$$

In addition, when $\sigma = 0$, then it follows from (6) and (30) that

$$H_{k+1}^{\text{SHS}} = \left(I - \frac{s_k y_k^T}{s_k^T y_k}\right) \left(I - \frac{y_k s_k^T}{s_k^T y_k}\right) \quad (35)$$

and $d_{k+1}^T g_{k+1} \leq 0$. Thus, the method defined by (1) and (5) with $\sigma = 0$ is the symmetric Hestenes-Stiefel method [18], denoted by SHS, which does not satisfy the descent property (7).

3 Scaling technology and restarting strategy

According to S.S. Oren and E. Spedicato's idea [20], D.F. Shanno applied the scaling technology to the memoryless BFGS update formula (31) and developed a self-scaling conjugate gradient algorithms [25], i.e., he translated the memoryless BFGS update formula (31) into

$$H_{k+1}(\rho) = \rho \left(I - \frac{s_k y_k^T + y_k s_k^T}{s_k^T y_k} + \frac{y_k^T y_k}{s_k^T y_k} \frac{s_k s_k^T}{s_k^T y_k} \right) + \frac{s_k s_k^T}{s_k^T y_k}. \quad (36)$$

Thus, the symmetric Perry matrix Q_{k+1} defined by (6) can be scaled as follows:

$$Q_{k+1}(\rho) = \rho \left(I - \frac{s_k y_k^T + y_k s_k^T}{s_k^T y_k} + \frac{y_k^T y_k}{s_k^T y_k} \frac{s_k s_k^T}{s_k^T y_k} \right) + \sigma \frac{s_k s_k^T}{s_k^T y_k}.$$

We substitute σ in $Q_{k+1}(\rho)$ with $\rho\sigma$, then $Q_{k+1}(\rho) = \rho Q_{k+1}$, where

$$\rho Q_{k+1} = \rho I - \rho \frac{s_k y_k^T + y_k s_k^T}{s_k^T y_k} + \left(\rho\sigma + \rho \frac{y_k^T y_k}{s_k^T y_k} \right) \frac{s_k s_k^T}{s_k^T y_k}. \quad (37)$$

Thus, the line search directions defined by (5) are rewritten as

$$\begin{cases} d_1 = -g_1, \\ d_{k+1} = -\rho Q_{k+1} g_{k+1} \\ \quad = -\rho g_{k+1} + \rho \frac{s_k^T g_{k+1}}{s_k^T y_k} y_k + \rho \left[\frac{y_k^T g_{k+1}}{s_k^T y_k} - \left(\sigma + \frac{y_k^T y_k}{s_k^T y_k} \right) \frac{s_k^T g_{k+1}}{s_k^T y_k} \right] s_k, \quad \forall k > 1, \end{cases} \quad (38)$$

from which a family of scaling Perry conjugate gradient methods can be deduced.

Based on Beale-Powell restarting strategy [24] (see also [2, 3, 25, 26]), we define the following scheme to compute the directions. When

$$|g_{r+1}^T g_r| \geq 0.2 \|g_{r+1}\|^2 \quad (39)$$

at r -th step, we use the directions defined by (38). For $k > r$, the directions d_{k+1} are computed by the following double update scheme:

$$d_{k+1} = -H_{k+1} g_{k+1} \quad (40)$$

with

$$H_{k+1} = H_{r+1} - \frac{s_k y_k^T H_{r+1} + H_{r+1} y_k s_k^T}{s_k^T y_k} + \left(\tilde{\sigma} + \frac{y_k^T H_{r+1} y_k}{s_k^T y_k} \right) \frac{s_k s_k^T}{s_k^T y_k} \quad (41)$$

and

$$H_{r+1} = \widehat{\rho} Q_{r+1} = \widehat{\rho} \left[I - \frac{s_r y_r^T + y_r s_r^T}{s_r^T y_r} + \left(\widehat{\sigma} + \frac{y_r^T y_r}{s_r^T y_r} \right) \frac{s_r s_r^T}{s_r^T y_r} \right], \quad (42)$$

where $\widetilde{\sigma}$, $\widehat{\rho}$ and $\widehat{\sigma}$ are three preset parameters.

Since

$$H_{r+1}^{-1/2} H_{k+1} H_{r+1}^{-1/2} = I - \frac{\widetilde{s}_k \widetilde{y}_k^T + \widetilde{y}_k \widetilde{s}_k^T}{\widetilde{s}_k^T \widetilde{y}_k} + \left(\widetilde{\sigma} + \frac{\widetilde{y}_k^T \widetilde{y}_k}{\widetilde{s}_k^T \widetilde{y}_k} \right) \frac{\widetilde{s}_k \widetilde{s}_k^T}{\widetilde{s}_k^T \widetilde{y}_k}, \quad (43)$$

where $\widetilde{s}_k = H_{r+1}^{-1/2} s_k$, $\widetilde{g}_{k+1} = H_{r+1}^{1/2} g_{k+1}$ and $\widetilde{y}_k = H_{r+1}^{1/2} y_k$, Corollary 1 asserts that $\kappa_2(H_{r+1}^{-1/2} H_{k+1} H_{r+1}^{-1/2})$ arrives at the minimum if $\widetilde{\sigma} = \frac{\widetilde{y}_k^T \widetilde{y}_k}{\widetilde{s}_k^T \widetilde{y}_k} = \frac{y_k^T H_{r+1} y_k}{s_k^T y_k}$. According to (42), Corollary 1 shows that $\kappa_2(H_{r+1})$ is minimal when $\widehat{\sigma} = \frac{y_r^T y_r}{s_r^T y_r}$. We also note that the matrix $H_{r+1}^{-1/2} H_{k+1} H_{r+1}^{-1/2}$ is similar to the matrix $H_{r+1}^{-1} H_{k+1}$, thus

$$\kappa_2(H_{k+1}) \leq \kappa_2(H_{r+1}) \kappa_2(H_{r+1}^{-1} H_{k+1}) = \kappa_2(H_{r+1}) \kappa_2(H_{r+1}^{-1/2} H_{k+1} H_{r+1}^{-1/2}), \quad (44)$$

which implies that the optimal choices for $\widetilde{\sigma}$ in (41) and $\widehat{\sigma}$ in (42) are

$$\widetilde{\sigma} = \frac{y_k^T H_{r+1} y_k}{s_k^T y_k} \text{ and } \widehat{\sigma} = \frac{y_r^T y_r}{s_r^T y_r}, \quad (45)$$

respectively, such that $\kappa_2(H_{k+1})$ is optimal.

Let $\widehat{g}_{k+1} = H_{r+1} g_{k+1}$ and $\widehat{y}_k = H_{r+1} y_k$, namely,

$$\widehat{g}_{k+1} = \widehat{\rho} g_{k+1} - \widehat{\rho} \frac{s_r^T g_{k+1}}{s_r^T y_r} y_r + \widehat{\rho} \left[\left(\widehat{\sigma} + \frac{y_r^T y_r}{s_r^T y_r} \right) \frac{s_r^T g_{k+1}}{s_r^T y_r} - \frac{y_r^T g_{k+1}}{s_r^T y_r} \right] s_r \quad (46)$$

and

$$\widehat{y}_k = \widehat{\rho} y_k - \widehat{\rho} \frac{s_r^T y_k}{s_r^T y_r} y_r + \widehat{\rho} \left[\left(\widehat{\sigma} + \frac{y_r^T y_r}{s_r^T y_r} \right) \frac{s_r^T y_k}{s_r^T y_r} - \frac{y_r^T y_k}{s_r^T y_r} \right] s_r, \quad (47)$$

then the directions d_{k+1} defined by (40) can be reformulated by

$$d_{k+1} = -\widehat{g}_{k+1} + \frac{s_k^T g_{k+1}}{s_k^T y_k} \widehat{y}_k - \left[\left(\widetilde{\sigma} + \frac{\widehat{y}_k^T \widehat{y}_k}{s_k^T y_k} \right) \frac{s_k^T g_{k+1}}{s_k^T y_k} - \frac{\widehat{y}_k^T g_{k+1}}{s_k^T y_k} \right] s_k. \quad (48)$$

Hence, we can introduce the following scaling symmetric Perry conjugate gradient method with restarting procedures (SSPCGRP).

Algorithm 2 (SSPCGRP)

Step 1. Give an initial point x_1 and $\varepsilon \geq 0$. Set $k = 1$ and Nrestart = 0.

Step 2. Calculate $g_1 = g(x_1)$. If $\|g_1\| \leq \varepsilon$, then stop, otherwise, let $d_1 = -g_1$.

Step 3. Calculate steplength α_k using the Wolfe line searches (15) and (16) with initial guess $\alpha_{k,0}$, where $\alpha_{1,0} = 1/\|g_1\|$ and $\alpha_{k,0} = \alpha_{k-1} \|d_{k-1}\|/\|d_k\|$ when $k \geq 2$.

- Step 4. Set $x_{k+1} = x_k + \alpha_k d_k$.
- Step 5. Calculate $g_{k+1} = g(x_{k+1})$. If $\|g_{k+1}\| \leq \varepsilon$ then stop.
- Step 6. If the Powell restarting criterion (39) holds, then calculate the directions d_{k+1} via (38) with different σ and ρ , let $y_r = y_k$ and $s_r = s_k$ (store y_r and s_r), set $N_{\text{restart}} = N_{\text{restart}} + 1$ and $k = k + 1$, go to step 3. Otherwise, go to step 7.
- Step 7. If $N_{\text{restart}} = 0$, then calculate the directions d_{k+1} via (38) with different σ and ρ , otherwise, calculate d_{k+1} via (48), where \hat{y}_k and \hat{g}_{k+1} are computed by (46) and (47), respectively, $\tilde{\sigma}$, $\hat{\sigma}$ and $\hat{\rho}$ are preset parameters.
- Step 8. Set $k = k + 1$, go to step 3.

In Algorithm 2, k and N_{restart} record the number of iterations and the number of restarting procedures, respectively.

When $\rho = 1$ and $\sigma = c_1 \frac{y_k^T y_k}{s_k^T y_k}$ in (38), and $\hat{\rho} = 1$, $\tilde{\sigma} = c_2 \frac{y_k^T H_{r+1} y_k}{s_k^T y_k}$ and $\hat{\sigma} = c_2 \frac{y_r^T y_r}{s_r^T y_r}$ in (46)–(48), then the SSPCGRP algorithm is denoted by SPDRP, or SPDRP(c_1, c_2) to indicate the dependence on the positive constants c_1 and c_2 . Especially, when they are equal to 1, i.e., $\sigma = \frac{y_k^T y_k}{s_k^T y_k}$ in (38), $\tilde{\sigma}$ and $\hat{\sigma}$ are computed by (45), the condition numbers $\kappa_2(Q_{k+1}) = \kappa_2(\rho Q_{k+1})$, $\kappa_2(H_{k+1})$ and $\kappa_2(H_{r+1})$ are optimal, where Q_{k+1} is defined by (6) with $\sigma = \frac{y_k^T y_k}{s_k^T y_k}$. So, the SSPCGRP algorithm is called the symmetric Perry descent conjugate gradient method with optimal condition numbers and restarting procedures, denoted by SPDOCRP.

When $\rho\sigma = 1$, $\rho = \frac{s_k^T s_k}{y_k^T s_k}$, $\hat{\rho}\hat{\sigma} = 1$, $\hat{\rho} = \frac{s_r^T s_r}{y_r^T s_r}$ and $\tilde{\sigma} = 1$, these formulas (38), (46), (47) and (48) were used by N. Andrei in [2], the SSPCGRP algorithm becomes the SCALCG algorithm with the spectral choice for θ_{k+1} [2], it is also called Andrei-Perry conjugate gradient method with restarting procedures.

4 Convergence

In this section, we analyze the convergence of the symmetric Perry conjugate gradient method (Algorithm 1) and the scaling symmetric Perry conjugate gradient method with restarting procedures (Algorithm 2). For this, we assume that the objective function $f(x)$ satisfies the following assumptions:

- H1. f is bounded below in \mathbb{R}^n and f is continuously differentiable in a neighborhood \mathcal{N} of the level set $\mathcal{L} \stackrel{\text{def}}{=} \{x : f(x) \leq f(x_0)\}$, where x_0 is the starting point of the iteration.
- H2. The gradient of f is Lipschitz continuous in \mathcal{N} , that is, there exists a constant $L > 0$ such that

$$\|\nabla f(\bar{x}) - \nabla f(x)\| \leq L \|\bar{x} - x\|, \quad \forall \bar{x}, x \in \mathcal{N}. \quad (49)$$

Next, we introduce the spectral condition lemma of the global convergence for an objective function satisfying H1 and H2, which comes from [18], Theorem 4.1.

Lemma 1 Let the objective function $f(x)$ satisfy H1 and H2. Assume that the line search directions of a nonlinear conjugate gradient method satisfy

$$d_1 = -g_1, d_k = -M_k g_k \quad \forall k > 1, \quad (50)$$

where M_k is the conjugate gradient iteration matrix, which is a symmetric positive semidefinite matrix. For a nonlinear conjugate gradient method (1) and (50) satisfying the sufficient descent condition (8), if its line search satisfies the Wolfe conditions (15) and (16), and

$$\sum_{k=1}^{\infty} (\Lambda_k)^{-2} = +\infty, \quad (51)$$

where Λ_k is the maximum eigenvalue of M_k , then $\liminf_{k \rightarrow \infty} \|g_k\| = 0$. Moreover, if $\Lambda_k \leq \tilde{\Lambda}$ for all k , where $\tilde{\Lambda}$ is a positive constant, then $\lim_{k \rightarrow \infty} \|g_k\| = 0$.

Remark 2 If M_k is a symmetric positive definite matrix, then the spectral condition (51) can be rewritten as

$$\sum_{k=1}^{\infty} (\kappa_2(M_k))^{-2} = +\infty. \quad (52)$$

In fact, by (50), it can be derived that

$$\cos^2 \theta_k = \frac{(g_k^T d_k)^2}{\|d_k\|^2 \|g_k\|^2} = \frac{(g_k^T M_k g_k)^2}{g_k^T M_k^T M_k g_k \|g_k\|^2} \geq \frac{\lambda_k^2 \|g_k\|^4}{\Lambda_k^2 \|g_k\|^4} = (\kappa_2(M_k))^{-2}, \quad (53)$$

where θ_k is the angle between d_k and $-g_k$, λ_k and Λ_k are the minimum eigenvalue and maximum eigenvalue of M_k , respectively. The Zoutendijk's condition (Theorem 2.1 of [8]) asserts that (52) implies that the results of Lemma 1 are true.

In what follows, the convergence of these resulting algorithms is proved by evaluating the spectral boundary of the iteration matrix and Lemma 1. The proof method is called the spectral method. It should be pointed out that the proof method also can be applied to the non-symmetric conjugate gradient methods, if the positive square root of the maximum eigenvalue $M_k^T M_k$ substitutes for with the one of M_k in Lemma 1, that is, the maximum singular value of M_k substitutes for the maximum eigenvalue of M_k (see Theorem 3.1 in [17]).

4.1 The convergence for uniformly convex functions

Here, we first prove the global convergence of the symmetric Perry conjugate gradient method (SPCG), the scheme (1) and (5) with Q_{k+1} defined by (6), for uniformly convex functions. For this, we introduce the following basic assumption, which is an equivalent condition for a uniformly convex differentiable function.

H3. There exists a constant $m > 0$ such that

$$(\nabla f(\bar{x}) - \nabla f(x))^T (\bar{x} - x) \geq m \|\bar{x} - x\|^2 \quad \forall \bar{x}, x \in \mathcal{N}. \quad (54)$$

Theorem 3 Assume that H1, H2 and H3 hold. Let v_0 and v_1 be two positive constants. For the symmetric Perry conjugate gradient method (1) and (5) with $v_0 \leq \sigma \leq v_1$, the Wolfe line searches (15) and (16) are implemented. If $g_1 \neq 0$ and steplength $\alpha_k > 0$ for $k \geq 1$, then $g_k = 0$ for some $k > 1$, or $\lim_{k \rightarrow \infty} \|g_k\| = 0$.

Proof Assume that $g_k \neq 0, \forall k \in \mathbb{N}$. Below, by induction, we first prove that the line search direction d_k , defined by (5), satisfies the sufficient descent property (8).

When $k = 1$, $d_1^T g_1 = -\|g_1\|^2 < 0$. From (16), it follows that $s_1^T y_1 \geq -(1 - b_2)\alpha_1 d_1^T g_1 > 0$.

Now, assume that $d_k^T g_k \leq -\frac{v_0 m}{L^2 + v_0 m} \|g_k\|^2$. Then, it follows from (16) that $s_k^T y_k \geq -(1 - b_2)\alpha_k d_k^T g_k > 0$. So, (30) and the assumptions H2 and H3 imply that

$$d_{k+1}^T g_{k+1} \leq -\frac{\sigma y_k^T s_k}{y_k^T y_k + \sigma y_k^T s_k} \|g_{k+1}\|^2 \leq -\frac{v_0 m}{L^2 + v_0 m} \|g_{k+1}\|^2.$$

Hence, by induction, the sufficient descent property (8) holds.

Next, we prove that $\lambda_{\max}^{(k+1)}$, the maximum eigenvalue of Q_{k+1} defined by (6), is uniformly bounded above. From the above analysis, it can be derived that $s_k^T y_k > 0$. So, from (23) in Theorem 2, it can be deduced that

$$\lambda_{\max}^{(k+1)} \leq \frac{y_k^T y_k s_k^T s_k}{(s_k^T y_k)^2} + \sigma \frac{s_k^T s_k}{s_k^T y_k} \leq \frac{L^2 \|s_k\|^4}{m^2 \|s_k\|^4} + \frac{\sigma \|s_k\|^2}{m \|s_k\|^2} = \frac{L^2}{m^2} + \frac{v_1}{m}. \quad (55)$$

Therefore, Lemma 1 claims that $\lim_{k \rightarrow \infty} \|g_k\| = 0$. \square

Remark 3 Theorem 3 shows that the memoryless BFGS quasi-Newton method and the method SPDCG are convergent for uniformly convex functions under the Wolfe line searches. In fact, the global convergence of the method SPDCG and the method mBFGS results from the following inequalities

$$m \leq \frac{y_k^T s_k}{s_k^T s_k} \leq \frac{y_k^T y_k}{s_k^T y_k} \leq \frac{L^2}{m}. \quad (56)$$

Next, we prove the global convergence of the SSPCGRP method for uniformly convex functions.

Theorem 4 Assume that H1, H2 and H3 hold, and that v_0 and v_1 are two positive constants. Let the sequence $\{x_k\}$ be generated by the SSPCGRP algorithm (Algorithm 2), where the five different parameters $\sigma, \rho, \tilde{\sigma}, \hat{\sigma}$ and $\hat{\rho}$ satisfy $v_0 \leq \sigma, \rho, \tilde{\sigma}, \hat{\sigma}, \hat{\rho} \leq v_1$. If $g_1 \neq 0$, and steplength $\alpha_k > 0$ for $k \geq 1$, then $g_k = 0$ for some $k > 1$, or $\lim_{k \rightarrow \infty} \|g_k\| = 0$.

Proof First, we note that $\tilde{y}_k^T \tilde{s}_k = y_k^T s_k$ for all $k \geq 1$. If $\tilde{y}_k^T \tilde{s}_k > 0$, we can denote the minimum and the maximum eigenvalues of the matrix $H_{r+1}^{-1/2} H_{k+1} H_{r+1}^{-1/2}$ by $\tilde{\lambda}_{\min}^{(k+1)}$ and $\tilde{\lambda}_{\max}^{(k+1)}$, respectively. We also denote the minimum and the maximum eigenvalues

of the matrix H_{r+1} by $\hat{\lambda}_{\min}^{(r+1)}$ and $\hat{\lambda}_{\max}^{(r+1)}$, respectively. Thus, (42), (43), Theorem 2 and the assumptions H2 and H3 imply that

$$\tilde{\lambda}_{\max}^{(k+1)} \leq \tilde{\omega}_k + \tilde{\sigma} \frac{\tilde{s}_k^T \tilde{s}_k}{\tilde{s}_k^T \tilde{y}_k}, \tilde{\lambda}_{\min}^{(k+1)} \geq \frac{\tilde{\sigma} \tilde{y}_k^T \tilde{s}_k}{\tilde{y}_k^T \tilde{y}_k + \tilde{\sigma} \tilde{y}_k^T \tilde{s}_k} \geq \frac{v_0 y_k^T s_k}{y_k^T H_{r+1} y_k + v_0 y_k^T s_k} \quad (57)$$

and

$$\hat{\lambda}_{\max}^{(r+1)} \leq \hat{\rho} \omega_r + \hat{\rho} \hat{\sigma} \frac{s_r^T s_r}{s_r^T y_r} \leq v_1 \frac{L^2 + v_1 m}{m^2}, \hat{\lambda}_{\min}^{(r+1)} \geq \frac{\hat{\rho} \hat{\sigma} y_r^T s_r}{y_r^T y_r + \hat{\sigma} y_r^T s_r} \geq \frac{v_0^2 m}{L^2 + v_0 m}, \quad (58)$$

where $\tilde{\omega}_k = \frac{\tilde{y}_k^T \tilde{s}_k \tilde{s}_k^T \tilde{s}_k}{(\tilde{s}_k^T \tilde{y}_k)^2}$ and $\omega_r = \frac{y_r^T y_r s_r^T s_r}{(s_r^T y_r)^2}$.

In what follows, by induction, we prove that $\tilde{y}_k^T \tilde{s}_k > 0$ and the sufficient descent property (8) is true for all k .

If the Powell restarting criterion (39) never holds for all $k \geq 1$, the iteration matrix is ρQ_{k+1} . Thus, similar to Theorem 3, it can be easily shown that the results of Theorem 4 are true.

Suppose that k_0 is the first natural number such that the Powell restarting criterion (39) is true, then $N_{\text{restart}} \geq 1$. Similar to Theorem 3, it can be obtained that for $k = 1, 2, \dots, k_0$, $\tilde{y}_k^T \tilde{s}_k = y_k^T s_k > 0$ and

$$d_{k+1}^T g_{k+1} \leq -\frac{\rho \sigma y_k^T s_k \|g_{k+1}\|^2}{y_k^T y_k + \sigma y_k^T s_k} \leq -\frac{\rho \sigma m \|g_{k+1}\|^2}{L^2 + \sigma m} \leq -\frac{v_0^2 m}{L^2 + v_0 m} \|g_{k+1}\|^2.$$

So, it follows from (16) and the above inequality that

$$s_{k+1}^T y_{k+1} \geq -(1 - b_2) \alpha_{k+1} d_{k+1}^T g_{k+1} > 0.$$

If the Powell restarting criterion (39) holds for $k + 2$, d_{k+2} is calculated by (38). Thus, Theorem 2 and the assumptions H2 and H3 claim that

$$d_{k+2}^T g_{k+2} \leq -\frac{\rho \sigma y_{k+1}^T s_{k+1} \|g_{k+2}\|^2}{y_{k+1}^T y_{k+1} + \sigma y_{k+1}^T s_{k+1}} \leq -\frac{\rho \sigma m \|g_{k+2}\|^2}{L^2 + \sigma m} \leq -\frac{v_0^2 m}{L^2 + v_0 m} \|g_{k+1}\|^2.$$

If the Powell restarting criterion (39) does not hold for $k + 2$, d_{k+2} is calculated by (48) with (46) and (47) (i.e., (40)–(42)). Since $N_{\text{restart}} \geq 1$, from (40)–(42) and Theorem 2, it can be obtained that

$$\begin{aligned} d_{k+2}^T g_{k+2} &= -g_{k+2}^T H_{k+2} g_{k+2} = -\tilde{g}_{k+2}^T H_{r+1}^{-1/2} H_{k+2} H_{r+1}^{-1/2} \tilde{g}_{k+2} \\ &\leq -\tilde{\lambda}_{\min}^{(k+2)} \tilde{g}_{k+2}^T \tilde{g}_{k+2} = -\tilde{\lambda}_{\min}^{(k+2)} g_{k+2}^T H_{r+1} g_{k+2} \leq -\tilde{\lambda}_{\min}^{(k+2)} \hat{\lambda}_{\min}^{(r+1)} \|g_{k+2}\|^2. \end{aligned}$$

By (57), (58), the assumptions H2 and H3, it is yielded that

$$\tilde{\lambda}_{\min}^{(k+2)} \geq \frac{v_0 y_{k+1}^T s_{k+1}}{\hat{\lambda}_{\max}^{(r+1)} \|y_{k+1}\|^2 + v_0 y_{k+1}^T s_{k+1}} \geq \frac{v_0 m^3}{(L^2 + v_1 m) v_1 L^2 + v_0 m^3}.$$

Therefore,

$$d_{k+2}^T g_{k+2} \leq -\frac{v_0^3 m^4 \|g_{k+2}\|^2}{(L^2 + v_0 m)((L^2 + v_1 m)v_1 L^2 + v_0 m^3)}$$

which, together with (16), implies that

$$s_{k+2}^T y_{k+2} \geq -(1 - b_2)\alpha_{k+2} d_{k+2}^T g_{k+2} > 0.$$

By induction, it follows that $s_k^T y_k > 0$ for all k and the directions generated by the SSPCRP algorithm (Algorithm 2) satisfy the sufficient descent property (8) with

$$c_0 = \min \left\{ \frac{v_0^2 m}{L^2 + v_0 m}, \frac{v_0^3 m^4}{(L^2 + v_0 m)((L^2 + v_1 m)v_1 L^2 + v_0 m^3)} \right\}.$$

Next, we prove that $\kappa_2(H_{k+1})$ is bounded above. Since $\tilde{s}_k = H_{r+1}^{-1/2} s_k$ and $\tilde{y}_k = H_{r+1}^{1/2} y_k$, from (57), (58) and the assumptions H2 and H3, it can be derived that

$$\begin{aligned} \tilde{\omega}_k &= \frac{\tilde{y}_k^T \tilde{y}_k \tilde{s}_k^T \tilde{s}_k}{(\tilde{s}_k^T \tilde{y}_k)^2} = \frac{y_k^T H_{r+1} y_k s_k^T H_{r+1}^{-1} s_k}{(s_k^T y_k)^2} \leq \frac{\hat{\lambda}_{\max}^{(r+1)} \omega_k}{\hat{\lambda}_{\min}^{(r+1)}} \leq \frac{(L^2 + v_0 m)(L^2 + v_1 m)}{v_0 m^3} \frac{L^2}{m^2}, \\ \tilde{\sigma} \frac{\tilde{s}_k^T \tilde{s}_k}{\tilde{s}_k^T \tilde{y}_k} &= \tilde{\sigma} \frac{s_k^T H_{r+1}^{-1} s_k}{s_k^T y_k} \leq \tilde{\sigma} \frac{s_k^T s_k}{\hat{\lambda}_{\min}^{(r+1)} s_k^T y_k} \leq v_1 \frac{L^2 + v_0 m}{v_0^2 m^2}, \\ \tilde{\lambda}_{\max}^{(k+1)} &\leq \frac{(L^2 + v_0 m)(L^2 + v_1 m)}{v_0 m^3} \frac{L^2}{m^2} + v_1 \frac{L^2 + v_0 m}{v_0^2 m^2} \end{aligned}$$

and

$$\tilde{\lambda}_{\min}^{(k+1)} \geq \frac{\tilde{\sigma} y_k^T s_k}{\hat{\lambda}_{\max}^{(r+1)} y_k^T y_k + \tilde{\sigma} y_k^T s_k} \geq \frac{v_0 m^3}{(L^2 + v_1 m)v_1 L^2 + v_0 m^3}.$$

Thus, it follows from (44), (58) and above two inequalities that

$$\kappa_2(H_{k+1}) \leq \frac{\hat{\lambda}_{\max}^{(r+1)} \tilde{\lambda}_{\max}^{(k+1)}}{\hat{\lambda}_{\min}^{(r+1)} \tilde{\lambda}_{\min}^{(k+1)}} \leq (L^2 + v_1 m)^3 \frac{((L^2 + v_1 m)v_1 L^2 + v_1 m^3)^2}{v_0^5 m^{11}}.$$

If d_{k+1} is calculated by (38), the iteration matrix is defined by (37). So, Corollary 1, (28), (29) and the assumptions H2 and H3 imply that

$$t = \left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right) / \left(2 \sqrt{\sigma \frac{s_k^T s_k}{y_k^T s_k}} \right) \leq \sqrt{\frac{m}{\sigma}} \frac{L^2 + \sigma m}{2m^2} \leq \sqrt{\frac{m}{v_0}} \frac{L^2 + v_1 m}{2m^2}$$

and

$$\kappa_2(\rho Q_{k+1}) = \kappa_2(Q_{k+1}) = \psi(t) \leq \psi \left(\sqrt{\frac{m}{v_0}} \frac{L^2 + v_1 m}{2m^2} \right),$$

where $\psi(\cdot)$ is defined by (29).

Hence, the spectral condition number of the iteration matrix of Algorithm 2 is uniformly bounded above, which claims that the results of Theorem 4 are true according to Remark 2. \square

From (56) and this theorem, it can be shown that the SPDRP algorithm and the SCALCG algorithm with the spectral choice [2] are global convergence for uniformly convex functions under the Wolfe line searches.

4.2 The convergence for general nonlinear functions

For general nonlinear functions, we first have following result for the symmetric Perry conjugate gradient method.

Theorem 5 Assume that H1 and H2 hold. For the symmetric Perry conjugate gradient method (1) and (5) with $\sigma = c \frac{y_k^T y_k}{s_k^T y_k}$, where c is a positive constant, if the line searches satisfy the Wolfe conditions (15) and (16), then $\lim_{k \rightarrow \infty} \|y_k\| = 0$ implies that $\liminf_{k \rightarrow \infty} \|g_k\| = 0$.

Proof Denote the maximum eigenvalue of the iteration matrix Q_{k+1} by $\lambda_{\max}^{(k+1)}$. The Wolfe condition (16) leads to $s_k^T y_k \geq -(1 - b_2)s_k^T g_k$, which, together with (33), implies that

$$\omega_k \leq \frac{y_k^T y_k s_k^T s_k}{(1 - b_2)^2 (-s_k^T g_k)^2} = \frac{y_k^T y_k g_k Q_k^2 g_k}{(1 - b_2)^2 (g_k P_k g_k) (-d_k^T g_k)} \leq \frac{(1 + c)\lambda_{\max}^{(k)} \|y_k\|^2}{(1 - b_2)^2 c \|g_k\|^2}. \quad (59)$$

Thus,

$$\lambda_{\max}^{(k+1)} \leq \omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} = (1 + c)\omega_k \leq \frac{(1 + c)^2 \lambda_{\max}^{(k)} \|y_k\|^2}{(1 - b_2)^2 c \|g_k\|^2} = \lambda_{\max}^{(k)} c_5^2 \frac{\|y_k\|^2}{\|g_k\|^2},$$

where $c_5 = \frac{1+c}{(1-b_2)\sqrt{c}}$. So,

$$\lambda_{\max}^{(k+1)} \leq \lambda_{\max}^{(k-1)} c_5^4 \frac{\|y_{k-1}\|^2}{\|g_{k-1}\|^2} \frac{\|y_k\|^2}{\|g_k\|^2} \leq \dots \leq \lambda_{\max}^{(1)} c_5^{2k} \prod_{j=1}^k \frac{\|y_j\|^2}{\|g_j\|^2}. \quad (60)$$

Now assume that $\lim_{k \rightarrow \infty} \|y_k\| = 0$, $\liminf_{k \rightarrow \infty} \|g_k\| = \varepsilon > 0$. Then there exists a positive integer N_0 such that for $j > N_0$, $\frac{\|y_j\|}{\|g_j\|} \leq c_5^{-1}$. Let $C_N = \lambda_{\max}^{(1)} \prod_{j=1}^{N_0} c_5^2 \frac{\|y_j\|^2}{\|g_j\|^2}$, thus,

$$\lambda_{\max}^{(k+1)} \leq \lambda_{\max}^{(1)} \prod_{j=1}^{N_0} c_5^2 \frac{\|y_j\|^2}{\|g_j\|^2} \prod_{j=N_0+1}^k c_5^2 \frac{\|y_j\|^2}{\|g_j\|^2} \leq C_N.$$

Therefore, Lemma 1 and (33) claim that $\lim_{k \rightarrow \infty} \|g_k\| = 0$, which contradicts the above assumption. So, $\lim_{k \rightarrow \infty} \|y_k\| = 0$ implies that $\liminf_{k \rightarrow \infty} \|g_k\| = 0$. \square

Next, we prove the global convergence of the SSPCGRP algorithm (Algorithm 2) for general nonlinear functions.

Theorem 6 Assume that H1 and H2 hold. Let the sequence $\{x_k\}$ be generated by the SSPCGRP algorithm with $\sigma = c \frac{y_k^T y_k}{s_k^T y_k}$ and $v_0 \leq \rho \leq v_1$ in (38), where c , v_0 and v_1 are positive constants. If the line searches satisfy the Wolfe conditions (15) and (16), then $\lim_{k \rightarrow \infty} \|y_k\| = 0$ implies that $\liminf_{k \rightarrow \infty} \|g_k\| = 0$.

Proof If $\liminf_{k \rightarrow \infty} \|g_k\| \neq 0$ as $\|y_k\| \rightarrow 0$, then, for some $\varepsilon > 0$, there exists a positive integer N_1 such that $\|g_{k+1}\| > \varepsilon$ and $\|y_k\| \leq 0.8\varepsilon$ as $k \geq N_1$. Thus,

$$\begin{aligned} \|g_{k+1}\|^2 &= g_{k+1}^T g_k + g_{k+1}^T y_k \leq g_{k+1}^T g_k + \|g_{k+1}\| \|y_k\| \\ &\leq g_{k+1}^T g_k + \|g_{k+1}\| 0.8\varepsilon \leq g_{k+1}^T g_k + 0.8\|g_{k+1}\|^2. \end{aligned}$$

So, $g_{k+1}^T g_k \geq 0.2\|g_{k+1}\|^2$ for $k \geq N_1$, which means that the directions d_{k+1} are calculated by (38) for $k \geq N_1$, that is,

$$d_{k+1} = -\rho Q_{k+1} g_{k+1},$$

where Q_{k+1} is defined by (6). Since $\sigma = c \frac{y_k^T y_k}{s_k^T y_k}$ and $v_0 \leq \rho \leq v_1$, from Theorem 2, it follows that

$$d_{k+1}^T g_{k+1} = -\rho g_{k+1}^T Q_{k+1} g_{k+1} \leq -\frac{\rho \sigma y_k^T s_k}{y_k^T y_k + \sigma y_k^T s_k} \|g_{k+1}\|^2 \leq -\frac{c v_0}{1+c} \|g_{k+1}\|^2. \quad (61)$$

For convenience, we also denote the maximum eigenvalue of ρQ_{k+1} by $\lambda_{\max}^{(k+1)}$. Analogous to (60), it can be derived that

$$\lambda_{\max}^{(k+1)} \leq \rho \left(\omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} \right) \leq v_1 c_5^2 \frac{\|y_k\|^2}{\|g_k\|^2} \lambda_{\max}^{(k)} \leq \dots \leq \lambda_{\max}^{(N_1)} \prod_{j=N_1}^k v_1 c_5^2 \frac{\|y_j\|^2}{\|g_j\|^2},$$

where $c_5 = \frac{1+c}{(1-b_2)\sqrt{c}}$. We substitute $\lambda_{\max}^{(N_1)}$ and N_1 for $\lambda_{\max}^{(1)}$ and 1 in (60), respectively, then, similar to Theorem 5, it can be obtained from Lemma 1 and (61) that $\lim_{k \rightarrow \infty} \|y_k\| = 0$ implies that $\liminf_{k \rightarrow \infty} \|g_k\| = 0$. \square

The above two theorems show that the SPDCG(c) algorithm and the SPDRP(c_1, c_2) algorithm are global convergence for the nonconvex functions under the Wolfe line searches, as $\lim_{k \rightarrow \infty} \|y_k\| = 0$. The condition for the global convergence, $\lim_{k \rightarrow \infty} \|y_k\| = 0$, was used by J.Y. Han, et al. in [14].

5 Numerical experiments

In this section, we demonstrate our algorithms: SPDCG and SPDRP, and compare them with the CG_DESCENT algorithm [12], the SCALCG algorithm with the spectral choice [2], the mBFGS algorithm (a special form of the SPCG algorithm with

$\sigma = 1$) and the RSPDCGs algorithm [19] whose line search directions are formulated by

$$d_1 = -g_1, \quad d_{k+1} = -g_{k+1} + \beta_k d_k, \quad k \geq 1,$$

where

$$\beta_k = \frac{1}{\eta_k^d} \left(y_k - \frac{\|y_k\|^2}{\eta_k^d} d_k \right)^T g_{k+1} \quad \text{with } \eta_k^d = \begin{cases} y_k^T d_k, & \text{if } \|g_k\|^2 \geq \eta \alpha_k \|d_k\|^2, \\ \alpha_k \|d_k\|^2, & \text{otherwise.} \end{cases} \quad (62)$$

In numerical experiments, we let $\eta = 10^{-5}$. The RSPDCGs algorithm is fully detailed in [19].

The numerical experiments use two groups test functions, one group (145 test functions) is taken from the CUTer [9] library, referring to website:

<http://www.cuter.rl.ac.uk/>,

which is only used to test mBFGS, SPDCG, RSPDCGs and CG_DESCENT algorithms. In order to compare with the SCALCG algorithm, the second group consists of the 73 unconstrained problems but the 71-st in SCALCG Fortran software package coded by N. Andrei, referring to website:

<http://camo.ici.ro/forum/SCALCG/>.

For the second group, each test function is made ten experiments with the number of variable 1000, 2000, ..., 10000, respectively. The starting points used are those given in the code, SCALCG.

The SPDCG, mBFGS and RSPDCGs algorithms are coded according to the package, CG_DESCENT (C language, Version 5.3), with minor revisions and implement the approximate Wolfe line searches with the default parameters in CG_DESCENT [10, 12]. The package, CG_DESCENT, can be got from Hager's web page at

<http://www.math.ufl.edu/~hager/>.

In addition, in order to compare with the SCALCG algorithm, all subroutines of the SPDRP algorithm are written in Fortran 77 with the double precision, and the SPDRP algorithm uses the Wolfe line searches in the SCALCG Fortran code.

The termination criterion of all algorithms is that $\|g\|_\infty < 10^{-6}$, where $\|\cdot\|_\infty$ is the infinity norm of a vector. The maximum number of iterations is $500n$, where n is the number of variables. The tests are performed on PC (Dell Inspiron 530), Intel® Core™ 2 Duo, E4600, 2.40 GHz, 2.39 GHz, RAM 2.00 GB, with the gcc and g77 compilers.

The SPDCG algorithm is a special form of the SPCG algorithm (Algorithm 1) with $\sigma = c \frac{y_k^T y_k}{s_k^T y_k}$ in (5) (see also step 6 in Algorithm 1). Thus the line search directions are formulated by

$$d_1 = -g_1, \quad d_{k+1} = -g_{k+1} + \beta_k d_k + \gamma_k y_k, \quad \forall k \geq 1 \quad (63)$$

with $\beta_k = \frac{y_k^T g_{k+1}}{d_k^T y_k} - (1+c) \frac{y_k^T y_k}{d_k^T y_k} \frac{d_k^T g_{k+1}}{d_k^T y_k}$, $\gamma_k = \frac{d_k^T g_{k+1}}{d_k^T y_k}$, and the iteration matrix is defined by (32). For the SPDCG algorithm, we test several different values of c in β_k of (63)

Fig. 1 Performance based on Nite of SPDOC, mBFGS, CG_DESCENT and RSPDCGs for large scale problems

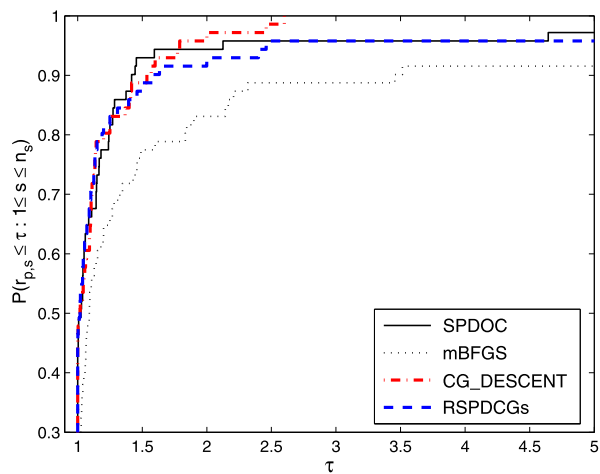
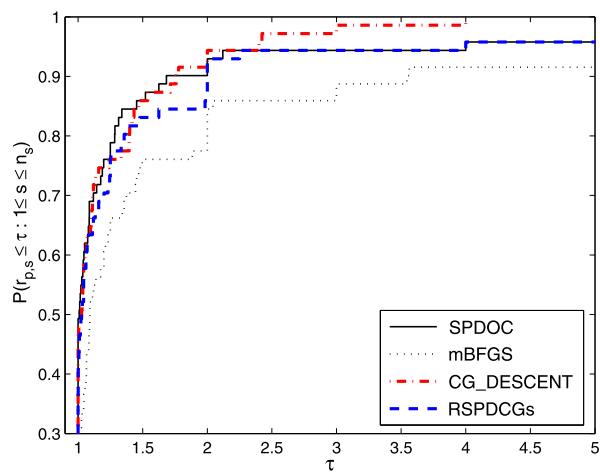


Fig. 2 Performance based on CPU time of SPDOC, mBFGS, CG_DESCENT and RSPDCGs for large scale problems



on the first group of test functions and find that the performance [6] is slightly better when $c = 1$ (SPDOC algorithm) than that when c is taken other values.

For the first group of test functions, to compare the algorithms: mBFGS and SPDOC with the RSPDCGs and CG_DESCENT algorithms, we divide the group into two parts: large scale problems, whose numbers of variables are not less than 100 (72 test functions), and small scale problems, whose numbers of variables are less than 100 (73 test functions).

Figures 1 and 2 present that their Dolan–Moré performance profiles for large scale problems based on Nite (the number of iterations) and CPU time, respectively. Figures 3 and 4 present the Dolan and Moré performance profiles of these algorithms for small scale problems with relative to Nite and CPU time, respectively. Figures 1 and 2 show that for large scale problems, the performance of the SPDOC algorithm is similar to that of the CG_DESCENT algorithm and their performances are better than that of the others; the performance of the RSPDCGs algorithm is better than

Fig. 3 Performance based on Nite of SPDOC, mBFGS, CG_DESCENT and RSPDCGs for small scale problems

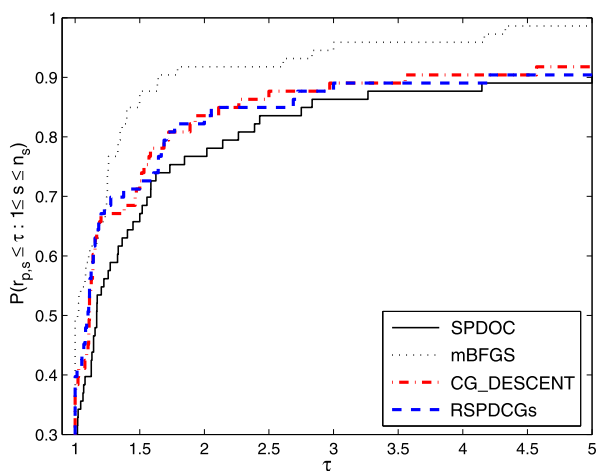
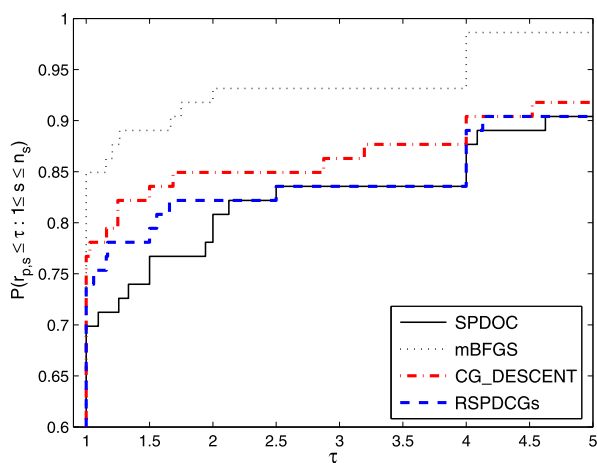


Fig. 4 Performance based on CPU time of SPDOC, mBFGS, CG_DESCENT and RSPDCGs for small scale problems



that of the mBFGS algorithm. For small scale problems, Figs. 3 and 4 show that the mBFGS algorithm is best, which means that SPDOC and CG_DESCENT algorithms are more suitable for solving large scale problems. It should be pointed out that although mBFGS algorithm give better results on the small problems, it fails to solve three problems of the CUTER test set. In the recent paper [13], it is observed that for the small ill-conditioned quadratic PALMER test problems in CUTER, the gradients generated by the conjugate gradient method quickly lose orthogonality due to numerical errors. See Hager and Zhang's paper [13] for a strategy for handling these ill-conditioned problems.

The SPDRP algorithm is a special case of the SSPCRP algorithm (Algorithm 2) with $\rho = 1$ and $\sigma = c_1 \frac{y_k^T y_k}{s_k^T y_k}$ in (38), and $\hat{\rho} = 1$, $\tilde{\sigma} = c_2 \frac{y_k^T H_{r+1} y_k}{s_k^T y_k}$ and $\hat{\sigma} = c_2 \frac{y_r^T y_r}{s_r^T y_r}$ in (46)–(48). For the SPDRP algorithm, we also test several different values of c on the second group of test functions, we find the performance is slightly better when $c_1 = c_2 = 1$ (i.e., the SPDOCRP algorithm) than that when c_1 and c_2 are taken other

Fig. 5 Performance based on Nite of SPDOCRP and SCALCG algorithms for the second group of test functions

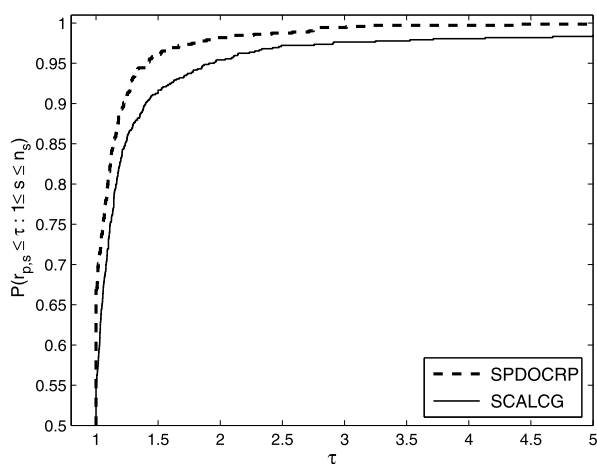
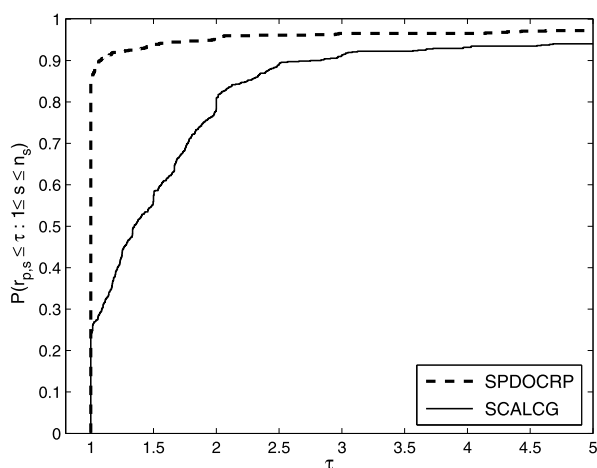


Fig. 6 Performance based on CPU time of SPDOCRP and SCALCG algorithms for the second group of test functions



values. Next, we compare the SPDOCRP algorithm with the SCALCG algorithms, using the second group of test functions. Figures 5 and 6 present that their Dolan-Moré performance profiles based on Nite and CPU time, respectively. The SPDOCRP algorithm and the SCALCG algorithm use the restarting strategy and the double update scheme, but the SPDOCRP algorithm has the optimal spectral condition number of the iteration matrix, so the SPDOCRP algorithm displays better numerical performance than the SCALCG algorithm.

So, the preliminary numerical experiments show that SPDOC and SPDOCRP are very effective algorithms for the large scale unconstrained optimization problems.

In addition, for the SPDCG algorithm, the inequality (33) shows that the descent degree of the line search directions of the algorithm becomes higher and higher as the value of c increases, but the performance of the algorithm is not directly proportional to c . In fact, the line search directions generated by the SPDCG algorithm vary with the value of c . What kind of criterion can be used to evaluate the performance of

an algorithm? Does the criterion exist? These are still open problems. Of course, the condition number and the descent property are two important factors.

In the end, it should be pointed out that the version 5.3 of CG_DESCENT (C code) uses a new formula for β_k ,

$$\beta_k = \frac{1}{y_k^T d_k} \left(y_k - \frac{\|y_k\|^2}{y_k^T d_k} d_k \right)^T g_{k+1}, \quad (64)$$

i.e., $\eta = 0$ in (62), instead of

$$\beta_k = \frac{1}{y_k^T d_k} \left(y_k - \frac{2\|y_k\|^2}{y_k^T d_k} d_k \right)^T g_{k+1},$$

presented in [10]. In [19], we proved that β_k formulated by (64) makes the spectral condition number of the iteration matrix defined by (4) with $u = s_k$ optimal.

6 Conclusion

In [18], we presented a rank one updating formula for the iteration matrix of the conjugate gradient methods:

$$M_{k+1} = M_{k+1}^{shs} + \frac{s_k \xi_k^T}{y_k^T \xi_k}, \quad \forall \xi_k \in \mathbb{R}^n,$$

where the symmetric Hestenes-Stiefel matrix M_{k+1}^{shs} is defined by

$$M_{k+1}^{shs} = \left(I - \frac{s_k y_k^T}{s_k^T y_k} \right) \left(I - \frac{y_k s_k^T}{s_k^T y_k} \right).$$

If we replace D_{k+1} with M_{k+1}^{shs} in (11), the symmetric Perry matrix (6) can be rewritten as

$$Q_{k+1} = M_{k+1}^{shs} + \sigma \frac{s_k s_k^T}{s_k^T y_k},$$

that is, if we apply the Powell symmetric technique to D_{k+1} in (11), we can obtain M_{k+1}^{shs} , then we add a rank one update $\sigma \frac{s_k s_k^T}{s_k^T y_k}$ to M_{k+1}^{shs} , we can also deduce the symmetric Perry matrix (6).

For the parameter σ in SPCG algorithm, besides the cases mentioned above, there also exist other choices, such as $\sigma = c^2 \frac{s_k^T s_k}{s_k^T y_k}$, $\sigma = c \frac{s_k^T y_k}{s_k^T s_k}$, $\sigma = c \frac{s_k^T y_k}{y_k^T y_k}$, $\sigma = c \frac{s_k^T s_k}{y_k^T y_k}$, $\sigma = c \frac{y_k^T y_k}{s_k^T s_k}$, and so on, where $c > 0$.

For the SSPCGRP algorithm, when $\rho\sigma = 1$, $\sigma = \frac{y_k^T y_k}{s_k^T y_k}$, $\hat{\sigma} = \frac{y_r^T y_r}{s_r^T y_r}$, $\hat{\rho} \hat{\sigma} = \tilde{\sigma} = 1$, these formulas (38), (46), (47) and (48) were suggested by D. F. Shanno in [25] and [26]. When $\rho = \sigma = \hat{\rho} = \tilde{\sigma} = \hat{\sigma} = 1$, the SSPCGRP algorithm becomes the

memoryless BFGS conjugate gradient method with restarting procedures. Therefore, it is worthy of studying further how the parameters σ and ρ are chosen to construct more effective nonlinear conjugate gradient algorithms.

The condition number of Q_{k+1} defined by (6) only depends on the parameter σ and the condition number of ρQ_{k+1} is the same as the one of Q_{k+1} (see (37)), so, we let $\rho = 1$ and $\hat{\rho} = 1$ in SSPCGRP algorithm. That is to say, σ can scale the symmetric Perry iteration matrix Q_{k+1} . Therefore, the symmetric Perry conjugate gradient methods have the self-scaling property. Similarly, σ can also alter the maximum and minimum eigenvalues of the Perry iteration matrix P_{k+1} defined by (4), and P_{k+1} is a self-scaling matrix. Thus, the parameter σ in the condition (12) is a self-scaling factor, which can alter the condition number of the iteration matrix of the conjugate gradient method.

From (30) and (23), we find that if we restrict that

$$|y_k^T s_k| > \delta \|s_k\|^2, \quad 0 < \delta < 1, \quad (65)$$

then under Lipschitz condition, $|y_k^T s_k| > \delta \|s_k\|^2 \geq \delta/L \|s_k\| \|y_k\|$, i.e., the angle between y_k and s_k is less than $\pi/2$. Thus,

$$d_{k+1}^T g_{k+1} \leq -\lambda_{\min}^{(k+1)} \|g_{k+1}\|^2 \leq -\frac{\sigma \delta}{L^2 + \sigma \delta} \|g_{k+1}\|^2 < 0$$

and

$$\lambda_{\max}^{(k+1)} \leq \omega_k + \sigma \frac{s_k^T s_k}{s_k^T y_k} = \frac{y_k^T y_k s_k^T s_k}{(s_k^T y_k)^2} + \sigma \frac{s_k^T s_k}{s_k^T y_k} \leq \frac{L^2}{\delta^2} + \frac{\sigma}{\delta}.$$

Therefore, according to Lemma 1, if a descent algorithm satisfies the condition (65), then it is globally convergent for nonconvex functions. So, (65) is also an interesting restarting strategy [19]. In fact, (65) is a uniformly convex condition.

Based on (6) and the relationship between the conjugate gradient method and quasi-Newton method, we let

$$\begin{aligned} H_{k+1} &= H_k - \frac{s_k y_k^T H_k + H_k y_k s_k^T}{s_k^T y_k} + \left(\sigma + \frac{y_k^T H_k y_k}{s_k^T y_k} \right) \frac{s_k s_k^T}{s_k^T y_k} \\ &= H_{k+1}^{\text{BFGS}} + (\sigma - 1) \frac{s_k s_k^T}{s_k^T y_k}, \end{aligned} \quad (66)$$

where

$$H_{k+1}^{\text{BFGS}} = H_k - \frac{s_k y_k^T H_k + H_k y_k s_k^T}{s_k^T y_k} + \left(1 + \frac{y_k^T H_k y_k}{s_k^T y_k} \right) \frac{s_k s_k^T}{s_k^T y_k}.$$

So, a new family of quasi-newton method can be obtained from (66), which belongs to Huang's family, but does not belongs to Broyden's family. Hence, it is worth probing further to develop new and more effective unconstrained optimization algorithms.

For example, we let $\sigma = c \frac{y_k^T H_k y_k}{s_k^T y_k}$ in (66).

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